Comment on "Efficiency of Isothermal Molecular Machines at Maximum Power"

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In recent Letter [1], efficiency of molecular machines is discussed by a one-state simple model. Where energy barrier position and number of stable state (s-state) are all assumed to be fixed. However, through calculations of molecular machines with specific expressions of energy potential, we found these assumptions are not generally true.

Assuming the energy potential is $U(x) = U_0(x) - (F_1 - F_2)x$, where F_1, F_2 are driving and loading forces respectively, $U_0(x)$ changes periodically with period L. Figs. 1(a, b) show, for the cases discussed in [1], energy barrier position λL changes with F_2. Moveover, Figs. 1(c, d) show number of s-state might also change with F_2. For large F_1 but small F_2, there is only one s-state (at $x = 0$ or L) and even $\lambda = 0$. With intermediate F_2, λ is nonzero but there is also one s-state. But for large F_2 there are two s-states, so one two-state model should be employed to calculate velocity V and power $\eta = F_2 V$ [2]. One consequence of increase of s-state number is that the velocity, and so the power, will decrease greatly. Figs. 2 (a, c) show, due to appearance of new energy barrier, η might not change smoothly with F_2. Meanwhile, due to the change of s-state number, maximal power η^* might also not change smoothly with F_1, see Fig. 2 (d).

Finally we remark that results obtained in [1] are right if potential $U_0(x)$ is piecewise linear or the driving force F_1 is small.

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[1] C. V. den Broeck, N. Kumar, and K. Lindenberg, Phys. Rev. Lett. **108**, 210602 (2012).

[2] M. E. Fisher and A. B. Kolomeisky, Proc. Natl. Acad. Sci. USA **96**, 6597 (1999).

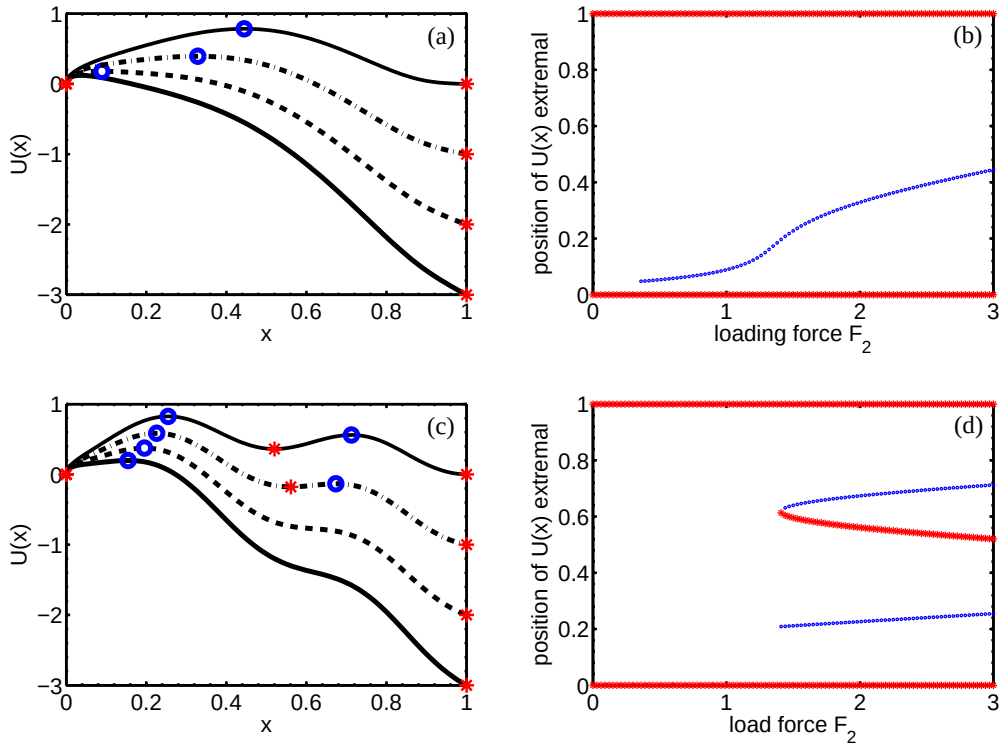

FIG. 1: The extremal points of potential $U(x) = U_0(x) - (F_1 - F_2)x$ change with loading force F_2 for $0 \leq F_2 \leq F_1 = 3$. For low loading force F_2, there might be only one state at $x = 0$ or L in one mechanochemical cycle, and no energy barrier for forward transition. For intermediate loading force F_2, there exists energy barrier for both forward and backward transitions. For high loading force F_2, molecular machine might have more than one state in one mechanical cycle (c, d). In the figures, maxima of potential $U(x)$ are marked with cycles, and minima are marked with asterisks. In (a, c), from the bottom up, the loading force used in the plots are $F_2 = 0, 1, 2, 3$ respectively.

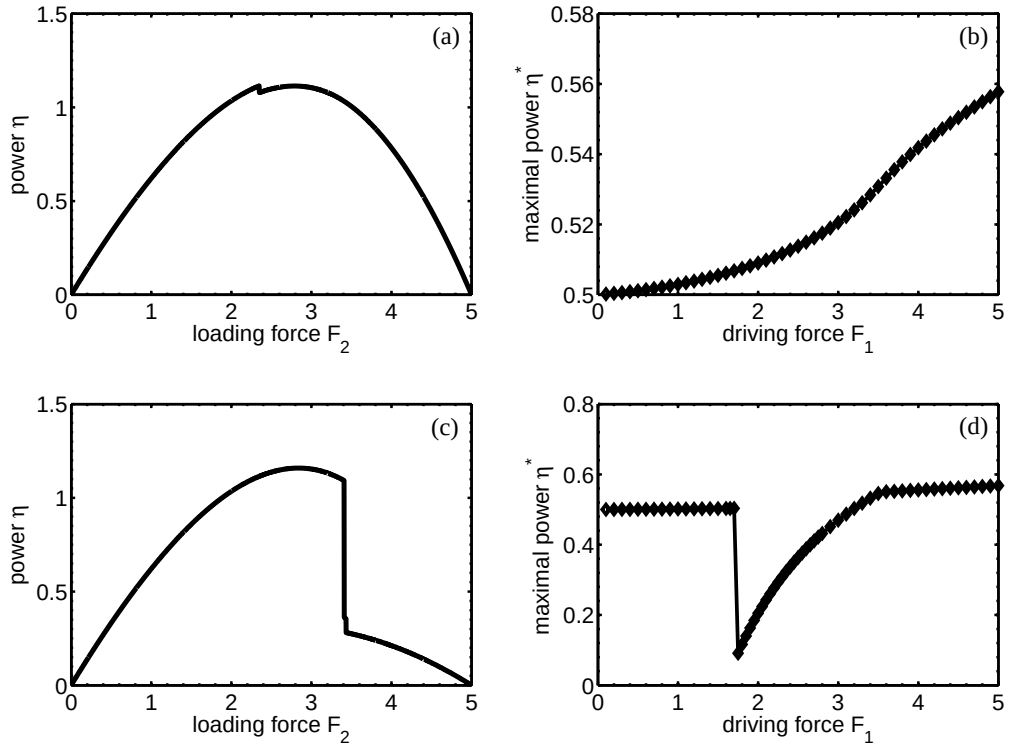

FIG. 2: The power $\eta = F_2/F_1$ (a, c) and its maximal value η^* (b, d) for one molecular machine with energy potential $U(x) = U_0(x) - (F_1 - F_2)x$. The function $U_0(x)$ used in (a, b) has only one maximum, and the one used in (c, d) has two maxima. In (a, c), the driving force used in the plots is $F_1 = 5$. The discontinuity of the curves in (a, c) is because one new maximum appears at the corresponding value of loading force F_2. The discontinuity of the curve in (d) is because for low driving force F_1 the molecular machine should be described by a two-state model [2], but for high driving force F_1 (and low loading force F_2) the molecular machine can be described by a one-state model [1].